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EMISSION CALCULATIONS FOR A SCRAMJET POWERED HYPERSONIC TRANSPORT

by Erwin A. Lezberg
Lewis Research Center
Cleveland, Ohio 44135
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ABSTRACT

Calculations of exhaust emissions from a scramjet powered hypersonic transport burning hydrogen fuel have been performed over a range of Mach numbers of 5 to 12 to provide input data for wake mixing calculations and forecasts of future levels of pollutants in the stratosphere.

The calculations were performed utilizing a one-dimensional chemical kinetics computer program for the combustor and exhaust nozzle of a fixed geometry dual-mode scramjet engine. Inlet conditions to the combustor and engine size was based on a vehicle of 2.27×10^5 kg (500 000 lb) gross take of weight with engines sized for Mach 8 cruise.

Nitric oxide emissions were very high for stoichiometric engine operation but for Mach 6 cruise at reduced equivalence ratio are in the range predicted for an advanced supersonic transport. Combustor designs which utilize fuel staging and rapid expansion to minimize residence time at high combustion temperatures were found to be effective in preventing nitric oxide formation from reaching equilibrium concentrations.

INTRODUCTION

Calculations of exhaust emissions from a scramjet powered hypersonic transport burning hydrogen fuel have been performed over a range of Mach numbers to provide input data for wake mixing calculations and forecasts of future levels of pollutants in the stratosphere.

There have been numerous studies of hypersonic transports over the past decade, but the introduction of such aircraft in commercial service is unlikely before 1990 or 2000. The Climatic Impact Assesment Program (CIAP) study of the Department of Transportation is concerned with long range predictions of the potential climatic effects of aircraft propulsion effluents in the upper atmosphere. Engine emission data similar to that available from current and advanced turbine engines are required for projections of a hypersonic transport fleet. The only published estimates of emissions for hypersonic aircraft known to the author are given in reference 1. These are based on equilibrium calculations at the combustor and nozzle exit. Chemical kinetic computer programs have been available for several years, and indeed have been utilized for scramjet engine performance predictions. Until recently however, the chemical reactions schemes have not included the nitrogen-oxygen and nitrogen-hydrogen-oxygen kinetics which are important to formation of the nitrogen oxides. This report presents the results of chemical kinetic calculations for a fixed geometry scramjet engine over the Mach number range of 5 to 12.

VEHICLE AND ENGINE CONFIGURATION

For purposes of engine sizing and geometry necessary for performing chemical kinetic calculations the following assumptions were made:

The vehicle accelerates from Mach 4 to Mach 6 using the dual-mode-scramjet engines in the subsonic burning mode. The vehicle can cruise at Mach 6 with supersonic combustion, or accelerate in the supersonic burning mode to Mach 8 cruise. Engines were initially sized for Mach 8 cruise but for purposes of this assesment of emissions, the calculations were extended to Mach 12. The all-body configuration assumed is taken from reference 2. The vehicle and engines were sized for a gross take off weight (GTOW) of 2.27×10^5 kg (0.5×10^6 lb). Since most studies are of hypersonic transports having a GTOW closer to 4.54×10^5 kg (10^6 lb), scaling of results may be necessary. The scramjet engines utilize an integrated modular configuration in which the forebody of the vehicle acts as a compression surface for the engine inlet and the aft surface as an extension of the exhaust nozzle. The vehicle trajectory was taken from reference 3 and is given in table 1. The altitude was limited by duct pressure for subsonic combustion below $M = 6$ and by aerodynamic heating above $M = 7$. The supersonic ramjet capture area was taken as 18.58 m^2 (200 ft^2) in the vehicle flow field. Range during the cruise portion of the flight at $M = 8$ is estimated to be 5315 km (2870 n. mi.), or a total range on the order of 10 000 km (5500 n. mi.).

The scramjet engines are arranged as eight side by side modules similar to the configuration described in reference 4. Compression from the vehicle forebody is assumed equal to a turning angle of 7.65°, half of which corresponds to the vehicle eliptical cone half angle and the remainder to angle of attack. In the extension of the calculations to $M = 12$, the angle of attack was reduced to zero to reduce the total compression ratio. This should not be construed as optimum in terms of vehicle aerodynamics but simply as an artifice to maintain constant geometry for the scramjet engine sized for $M = 8$ cruise.

Inlet Assumptions

The module inlet consists of a 6° ramp followed by lateral compression by the module dividers and turning by the module cowl to the free stream direction. Total pressure losses are determined by the vehicle forebody, 6° ramp, and cowl shocks. For subsonic combustion, an additional normal shock is assumed. The lateral compression by the module dividers with a contraction ratio of 2.9 is assumed to be isentropic. Full capture of the air compressed by the 6° ramp is assumed at $M = 8$ with spillage through a serrated cowl at Mach numbers below 8. Air flow rate captured by the inlet and fuel flow ratios based on equivalence ratios of 0.65, 1.0 and 1.5 are given in table 1.

Combustor Geometry

The combustor area ratio (combustor exit area/combustor inlet area) for a scramjet affects the performance and low Mach number thermal choking. In addition, for kinetic calculations, the static temperature of the fuel air mixture determines whether ignition can be initiated before expansion to a larger area quenches the preignition reactions. In order to perform the kinetic calculations, the combustor area ratio at which fuel is introduced was varied with flight Mach number to prevent thermal choking and insure ignition. The combustor geometry is shown schematically in figure 1. The entrance consists of a rectangular duct of 0.533 m (1.75 ft) height and 0.818 m (2.68 ft) width. The combustor expands laterally with a 4° half angle. Sudden step increases in area to area ratios of 1.5 and 2.75 are provided for second stage fuel injection and to prevent thermal choking at the lower flight Mach numbers. A fourteen degree half angle expansion section is provided as the initial portion of the exhaust nozzle. Combustor length was cut off at the maximum static temperature (completion of combustion) and matched to the nozzle area at that location. In practice, fuel staging and diffusion controlled combustion can be used to limit thermal choking, control combustor length and therefore minimize engine cooling requirements.

CHEMICAL KINETIC CALCULATIONS

The scramjet combustor kinetic calculations were performed using the computer program described in reference 5. The set of reactions and rate constants used in the analysis are given in the appendix. The combustor inlet conditions given in table 2 were modified by a mass and energy balance with injected fuel. Fuel temperature was assumed to be at 700 K or 1000 K after cooling the engine. For calculations where fuel staging was used, the calculations were restarted with a new mass and energy balance after adding the second stage fuel. Step increases in area could not be accommodated by the computer program, and the calculations were restarted by using the one-dimensional isentropic relationships with constant gamma for reinitializing conditions. Starting conditions for the cases run with the computer program are given in table 3.

For Mach 6 combustor calculations, ignition did not occur at the fuel-air mixture temperature. The temperature was arbitrarily increased to 1150 K to achieve ignition, and the enthalpy of the combustion products following first stage combustion then decreased by the same amount which was required to bring the reactants to 1150 K. Since only small amounts of NO were formed during the first stage combustion at an equivalence ratio of 0.3, this piloting simulation would not be expected to affect the exhaust emissions.

RESULTS AND DISCUSSION

Increase of nitric oxide concentration in the combustor and freezing during the initial nozzle expansion is shown in figure 2 over the Mach number range of 5 to 12. Following the ignition delay, the nitric oxide growth increases rapidly with combustion temperature but lags the equilibrium value at the local temperature. The sudden decrease in nitric oxide composition following first stage injection, (figs. 2(a), (b), and (c)), are due to the readjustment of the composition following the introduction ofsecond stage fuel. Initially, following cutoff of the combustor and initiation of the 14° half angle expansion, nitric oxide continues to increase and approach equilibrium at the local static temperature but is eventually frozen during expansion. At the expansion angle chosen, it was not possible to freeze the nitric oxide concentration at the maximum temperature location (complete combustion). Practically, much larger expansion angles would result in nozzle performance losses.

A possible operating mode for hypersonic cruise at Mach 6 would be to throttle the fuel to an equivalence ratio below stoichiometric. If the lower fuel flow were adequate to cool the engine and aircraft as noted in reference 6, then it should be possible to increase payload or range by decreasing cruise altitude to increase vehicle lift-drag ratio (ref. 2). Note that the fixed geometry engine considered was sized for Mach 8 cruise and hence would be oversize for Mach 6 cruise for the acceleration trajectory shown in table 1. Figure 2(a), shows the nitric oxide growth in the combustor and nozzle for an equivalence ratio of 0.65. Maximum values are comparable to projected ASST levels (ref. 7), but considerably below the levels indicated for stoichiometric operation.

The kinetic calculations reported herein assume instantaneous mixing and exhibit finite ignition delays. In the other extreme of diffusion controlled combustion, the reaction occurs instantaneously forming equilibrium products at a postulated flame sheet which is located at the stoichiometric mixing plane. In the real case, a diffusion flame will result unless the ignition delay is long enough to allow sufficient premixing to reduce mixture composition everywhere below stoichiometric. The implication with respect to nitric oxide formation is that the reactants in a diffusion flame diffuse and react in the flame zone at near stoichiometric temperatures. The kinetics of nitric oxide formation will be governed by the time-temperature history of stream tubes passing through the flame front and hence concentrations may be higher than indicated by the present calculations.

Figure 2(d) shows a comparison at Mach 10 of nitric oxide growth at $\varphi = 1$ and 1.5. Operation at an equivalence ratio greater than 1.0 may be necessary to cool the engine and aircraft and will result in performance penalties. The reduction in NO by a factor of 2.7 reflects the stoichiometry since maximum combustion temperatures differ only by 20 K (table 4).

Results of nitric oxide formation with subsonic combustion at M = 5 flight conditions are shown in figure 2(f). The combination of high combustion temperature and long residence time for subsonic combustion produced nitric oxide concentrations close to equilibrium values.

A thermal throat was simulated by isentropically expanding the flow to slightly supersonic conditions (M = 1.07) from the combustor maximum temperature location followed by a 14° kinetic expansion. Nitric oxide concentration was frozen at a level considerably below equilibrium.

Figure 3 shows combustion temperature profiles as a function of combustor geometry and fuel staging for the M = 8, flight condition. When all the fuel is added in the first stage in a slowly diverging combustor (Case 1), peak combustion temperatures are reached very rapidly, and the nitric oxide concentration reaches the equilibrium value of about 10 000 ppm in less than 80 cm. Fuel staging and increase in combustor area is effective in reducing nitric oxide formation by decreasing the residence time at the combustion temperature.

The results of a chemical kinetic expansion through the 14° half angle exhaust nozzle are shown in figure 4, where species mole fraction is plotted against distance from the nozzle entrance. Combustor exit and nozzle exit conditions for the kinetic calculations are given in table 4. The nozzle calculations were terminated at a nozzle exit to combustor inlet area ratio of 6.17. The expansion along the aft surface of the vehicle will continue to the point where the static pressure matches the flow field pressure or until the flow separates. Certain of the species which may be of importance to upper atmosphere chemistry (OH, O, H) are continuing to decay at the point where the calculations were terminated but nitric oxide has frozen early during the expansion. The other oxides of nitrogen are present in insignificant amounts.

The emissions at the nozzle exit are given in table 5 in terms of the emission index. Total flow rates for each specie for the total engine are also indicated. These values can probably be scaled directly by GTOW for aircraft GTOW other than 2.27×10^{5} kg (0.5×10^{6} lb), and for change in altitude, since combustor length will remain relatively constant with modular design and nitric oxide formation should be reasonably insensitive to pressure.

CONCLUDING REMARKS

Kinetic calculations were performed for a scramjet combustor and nozzle sized to propell a hypersonic aircraft at Mach 8 cruise. Calculations were made over a range of Mach numbers from 5 to 12 to provide values for exhaust emissions at high altitudes. Nitric oxide emissions were very high for stoichiometric engine operation but for Mach 6 cruise at reduced equivalence ratio are in the range predicted for an advanced supersonic transport. Combustor designs which utilize fuel staging and rapid expansion to minimize residence time at high combustion temperatures can be effective in reducing nitric oxide since its formation is a strong function of combustion temperatures.

APPENDIX - REACTIONS AND RATE CONSTANTS

$[K = AT^N \exp(E/RT)\ \mathrm{cm^3\ mole^{-1}\ sec^{-1}}$ or $\mathrm{cm^6\ mole^{-2}\ sec^{-1}}.]$

REACTION NUMBER	REACTION							REACTION RATE VARIABLES A	N	ACTIVATION ENERGY
1	N	+	O	=	NO	+	M	6.44000E+16	-0.5000	0.
2	N_2O	+	O	=	NO	+	NO	2.50000E+13	0.	26900.00
3	N	+	NO	=	N_2	+	O	3.10000E+13	0.	334.00
4	N	+	O_2	=	NO	+	O	6.40000E+09	1.0000	6250.00
5	N_2O	+	O	=	N_2	+	O_2	2.50000E+13	0.	26900.00
6	NO	+	HO_2	=	NO_2	+	OH	1.00000E+13	0.	2380.00
7	NO_2	+	H	=	NO	+	OH	7.20000E+14	0.	1930.00
8	O	+	NO_2	=	NO	+	O_2	5.50000E+12	0.	0.
9	NO	+	O	=	NO_2	+	M	9.40000E+14	0.	-1930.00
10	N	+	OH	=	NO	+	H	4.00000E+13	0.	0.
11	H_2	+	O_2	=	H_2O	+	O	4.10000E+13	0.	50400.00
12	M	+	O_2	=	O	+	O	2.75000E+19	-1.0000	118700.00
13	H	+	O_2	=	OH	+	O	1.25000E+14	0.	16300.00
14	H	+	O_2	=	HO_2	+	M	1.59000E+15	0.	-1000.00
15	O	+	H_2	=	OH	+	H	2.96000E+13	0.	9800.00
16	H_2	+	OH	=	H_2O	+	H	2.10000E+13	0.	5100.00
17	H	+	H	=	H_2	+	M	1.00000E+18	-1.0000	0.
18	H	+	OH	=	H_2O	+	M	7.50000E+23	-2.6000	0.
19	H	+	HO_2	=	OH	+	OH	7.00000E+13	0.	0.
20	HO_2	+	OH	=	H_2O	+	O_2	6.00000E+12	0.	0.
21	HO_2	+	O	=	OH	+	O_2	6.00000E+12	0.	0.
22	O	+	H_2O	=	OH	+	OH	5.75000E+13	0.	18000.00

ALL THIRD BODY RATIOS ARE 1.0 EXCEPT THE FOLLOWING

M(O ,12) = 3.00000	M(N2 , 9) = 1.55000	M(N2 ,14) = 2.00000	M(N2 ,17) = 1.50000
M(N2 ,18) = 1.60000	M(O2 ,14) = 2.00000	M(O2 ,17) = 1.50000	M(O2 ,18) = 1.60000
M(H2 , 1) = 2.25000	M(H2 ,14) = 5.00000	M(H2 ,17) = 4.00000	M(H2 ,18) = 4.00000
M(H2O , 1) = 6.80000	M(H2O , 9) = 6.30000	M(H2O ,14) = 22.50000	M(H2O ,17) = 15.00000
M(H2O ,18) = 20.00000			

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TABLE 1. - HYPERSONIC VEHICLE TRAJECTORY AND MASS THROUGHPUT

(2.27×10^5 kg GTOW)

Flight Mach Number	Altitude		Air flow rate		Fuel flow rate kg/sec		
	m	ft	kg/sec	lb/sec	$\varphi = .65$	1.0	1.5
5	21340	70 000	2.902×10^3	6.393×10^3	------	84.62	------
6	27430	90 000	1.648×10^3	3.629	31.23	48.05	------
7	32920	108 000	9.95×10^2	2.193	------	29.01	------
8	36580	120 000	7.29	1.606	------	21.26	------
10	39620	130 000	4.85	1.068	------	14.14	21.21
12	42670	140 000	4.05	8.918×10^2	------	------	17.71

TABLE 2. - COMBUSTOR INLET CONDITIONS

Flight Mach Number	5	6	7	8	10	12
Pressure, atm	12.4	2.59	1.263	0.957	0.674	0.690
Temperature, ^{o}K	1222	972	1144	1333	1469	1814
Velocity, m/sec	431	1260	1540	1980	2494	2804

TABLE 3. - FUEL-AIR MIXTURE CONDITIONS FOR KINETIC CALCULATIONS

Flight Mach number	5	6	6	7	7	8	8	10	10	12
Stage	Subsonic	1	2	1	2	1	2	1	1	1
Area ratio	1.0	1.0	2.75	1.0	1.5	1.0	1.5	1.0	1.0	1.0
Equivalence ratio	1.0	0.3	0.65	0.3	1.0	0.3	1.0	1.0	1.5	1.5
Pressure, atm	12.4	2.59	.93	1.26	1.315	0.957	0.927	0.674	----	0.69
Temperature, K	1161	[a]1150	[b]1359	1100	1585	1270	1686	1341	1301	1523
Velocity, m/sec	431	1260	1562	1540	1812	1980	2316	2494	----	2804
Fuel temperature, K	1000	700	700	700	700	700	700	1000	----	1000

[a]Enthalpy increased by 1616.09 Cal/mole to ignite mixture.

[b]Enthalpy decreased by 1616.09 Cal/mole to adjust for correct reaction temperature.

TABLE 4. - SCRAMJET MODULE

[Combustor and nozzle exit conditions (AR = 6.17).]

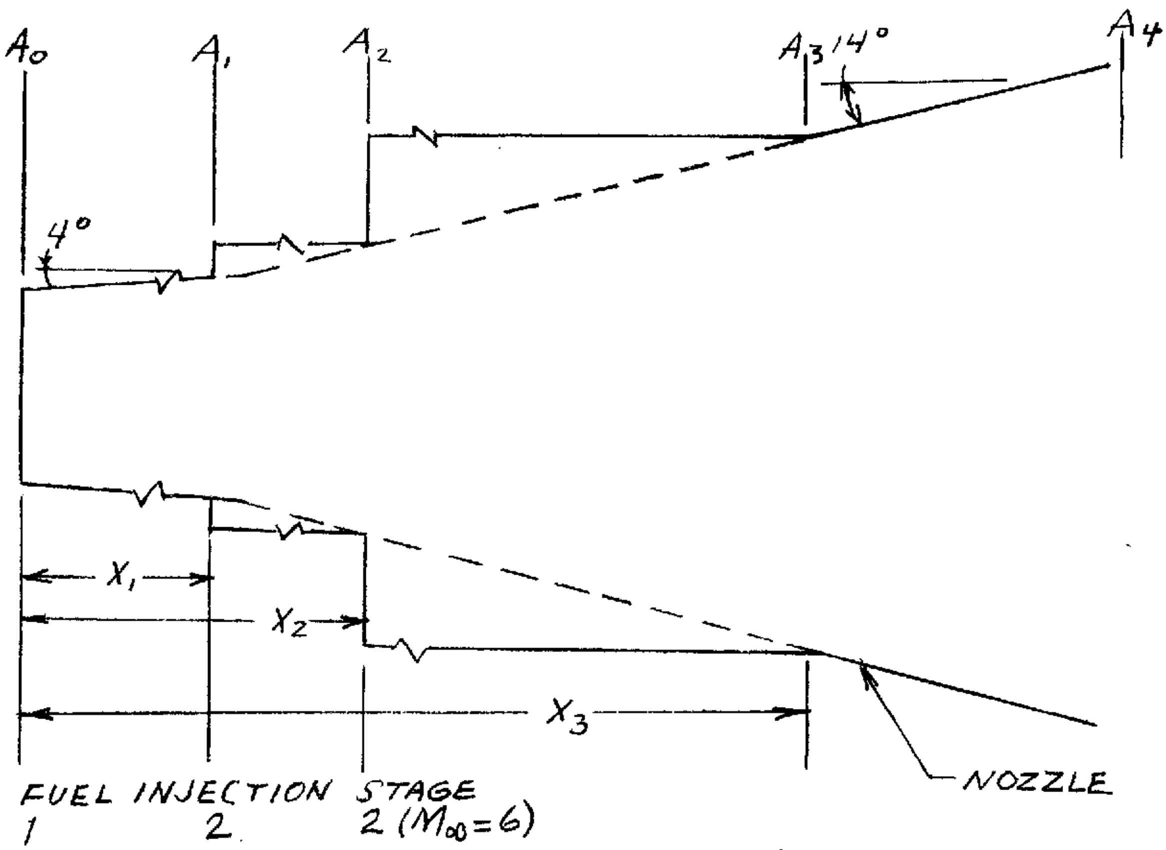
Flight Mach number	5	6	7	8	10	10	12
Equivalence ratio	1.0	0.65	1.0	1.0	1.0	1.5	1.5
Pressure,[a] atm	7.417	1.971	3.041	1.638	1.306	1.386	1.18
	0.471	0.439	0.273	0.212	0.120	0.118	0.111
Temperature,[a] K	2717	2414	2952	2893	2907	2928	2953
	1704	1809	2066	2150	2068	1996	2075
Velocity,[a] m/sec	1080.6	1282	1354	2092	2288	2238	2627
	2312	1917	2502	2859	3073	3147	3425
Mach number[a]	1.0	1.296	1.158	1.802	1.995	1.828	2.124
	2.703	2.23	2.586	2.885	3.216	3.139	3.339
Gamma	1.244	1.258	1.250	1.251	1.256	1.256	1.258
	1.264	1.271	1.257	1.257	1.261	1.266	1.266
Molecular weight[a]	24.07	25.78	22.44	22.33	23.07	20.38	20.19
	24.48	25.87	23.06	22.87	23.75	20.90	20.76

[a] $\frac{\text{Combustor}}{\text{Nozzle}}$

TABLE 5. - HYPERSONIC VEHICLE EFFLUENT

[Mass throughput, 2.27×10^5 kg GTOW]

Flight Mach number	5	6	7	8	10	10	12
Equivalence ratio	1.0	0.65	1.0	1.0	1.0	1.5	1.5
Constituent:							
NO							
g/kg fuel	85.15	42.5	212	205	306	87.2	111
kg/sec	7.20	1.33	6.15	4.35	4.33	1.85	1.95
H_2O							
g/kg fuel	8798	8912	8709	8518	7680	5840	5740
kg/sec	744	278	252	181	108	124	101
OH							
g/kg fuel	38.1	106	104	198	333	92.5	142
kg/sec	3.22	3.33	3.02	4.20	4.70	1.96	2.51
H_2							
g/kg fuel	19.1	3.15	191	204	105	320	317
kg/sec	1.62	.098	5.54	4.33	1.48	6.78	5.61
O_2							
g/kg fuel	123	4252	36.5	103	667	20.0	39.8
kg/sec	10.4	133	1.06	2.19	9.43	.424	.705
O							
g/kg fuel	2.63	15.1	16.4	51.4	95.0	11.2	25.7
kg/sec	.222	.473	.35	1.1	1.34	.238	.455
H							
g/kg fuel	.854	.301	10.9	19.6	21.8	27.5	37.1
kg/sec	.007	.009	.31	.417	.308	.585	.657



Area Ratio	$A_1/A_o = 1 + 2.55 \times 10^{-3} X_1$	$A_2/A_o = 1.5$	$A_3/A_o = 2.75$
	Distance from Combustor Entrance		
M_∞	X_1	X_2	X_3 2cm
5	50	56*	
6	8	50	180
7	50	60	
8	50	90	
10	42		
12	42		

*Area ratio at sonic throat = 1.36

FIG. 1. SCHEMATIC OF COMBUSTOR GEOMETRY

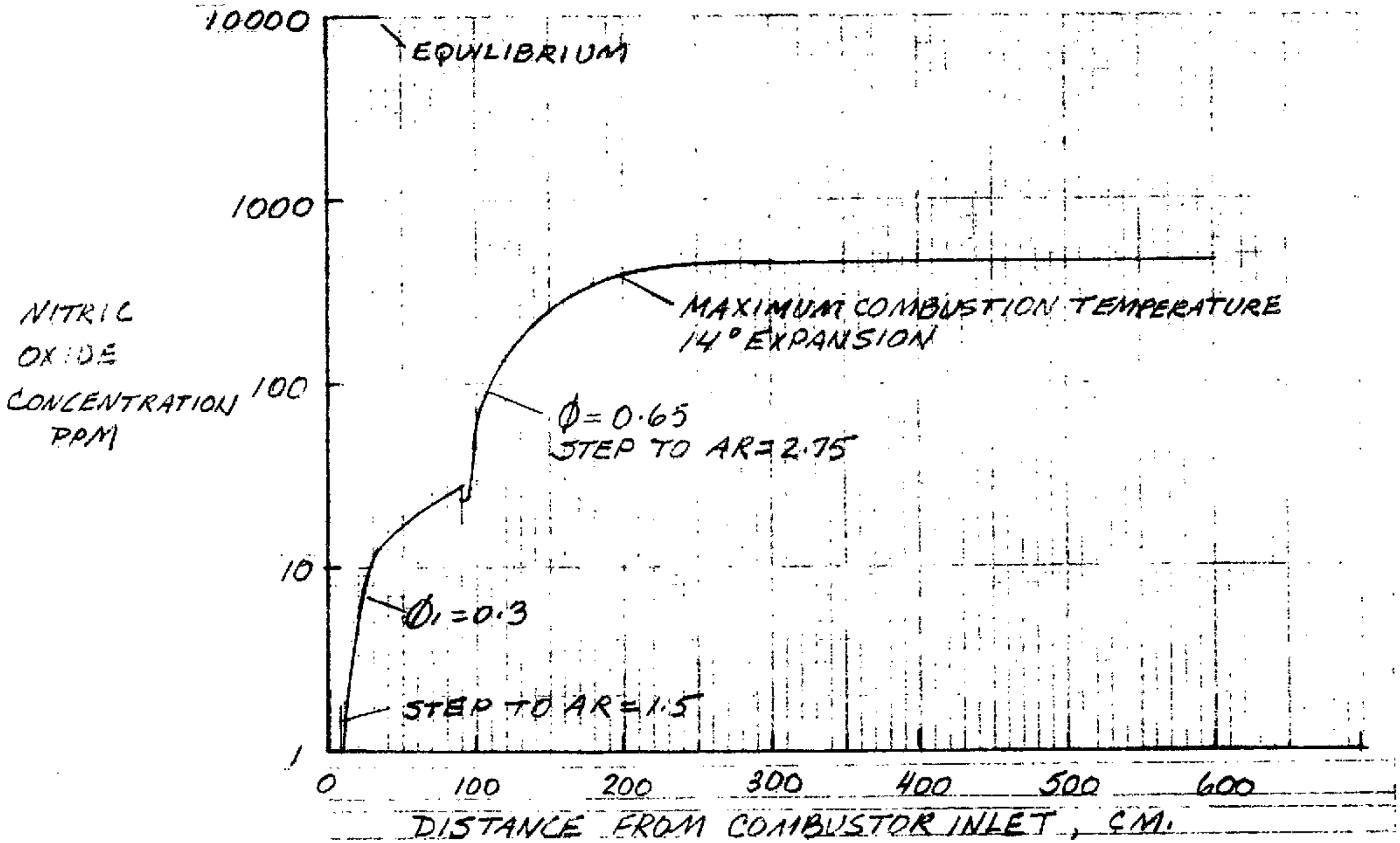
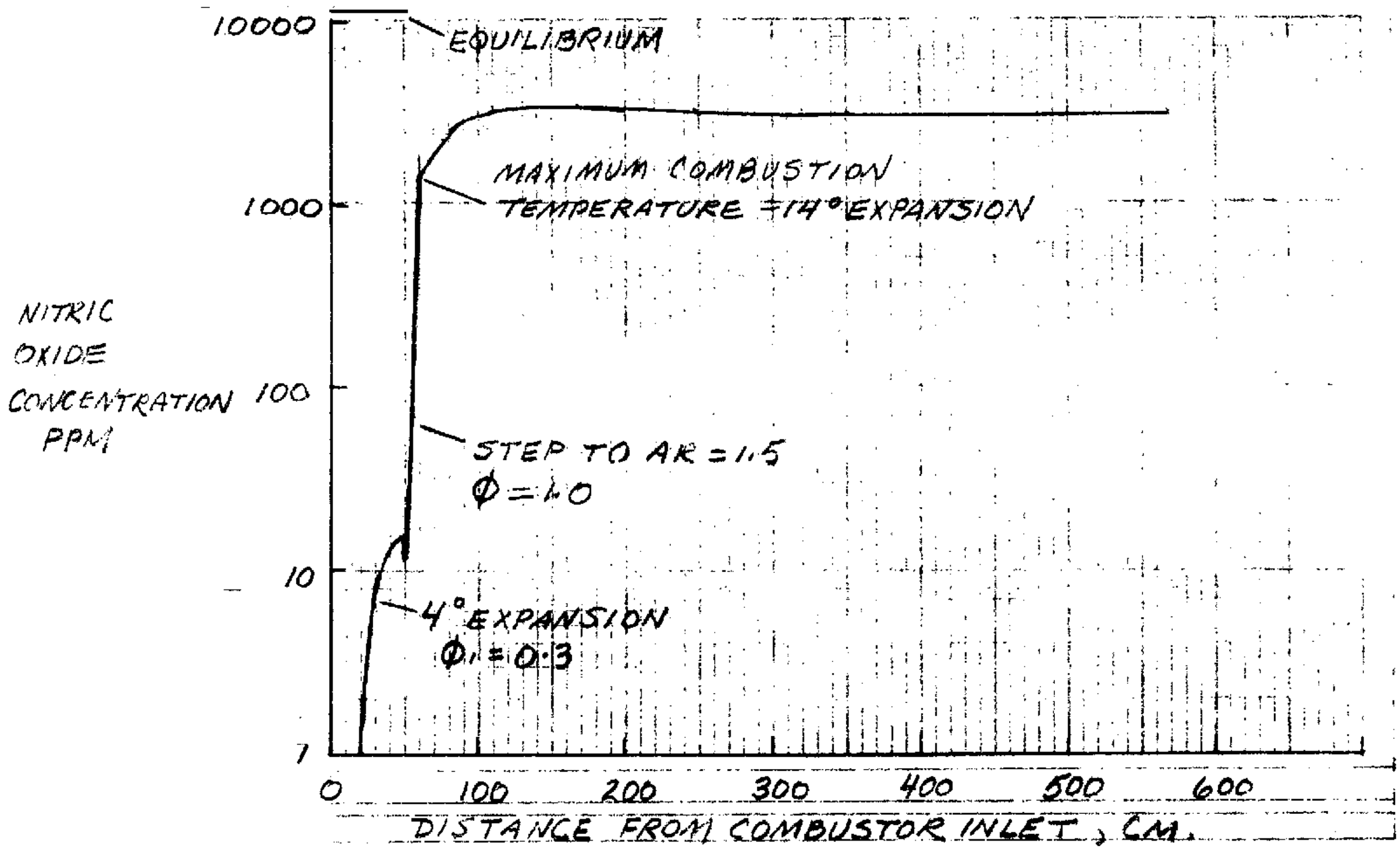
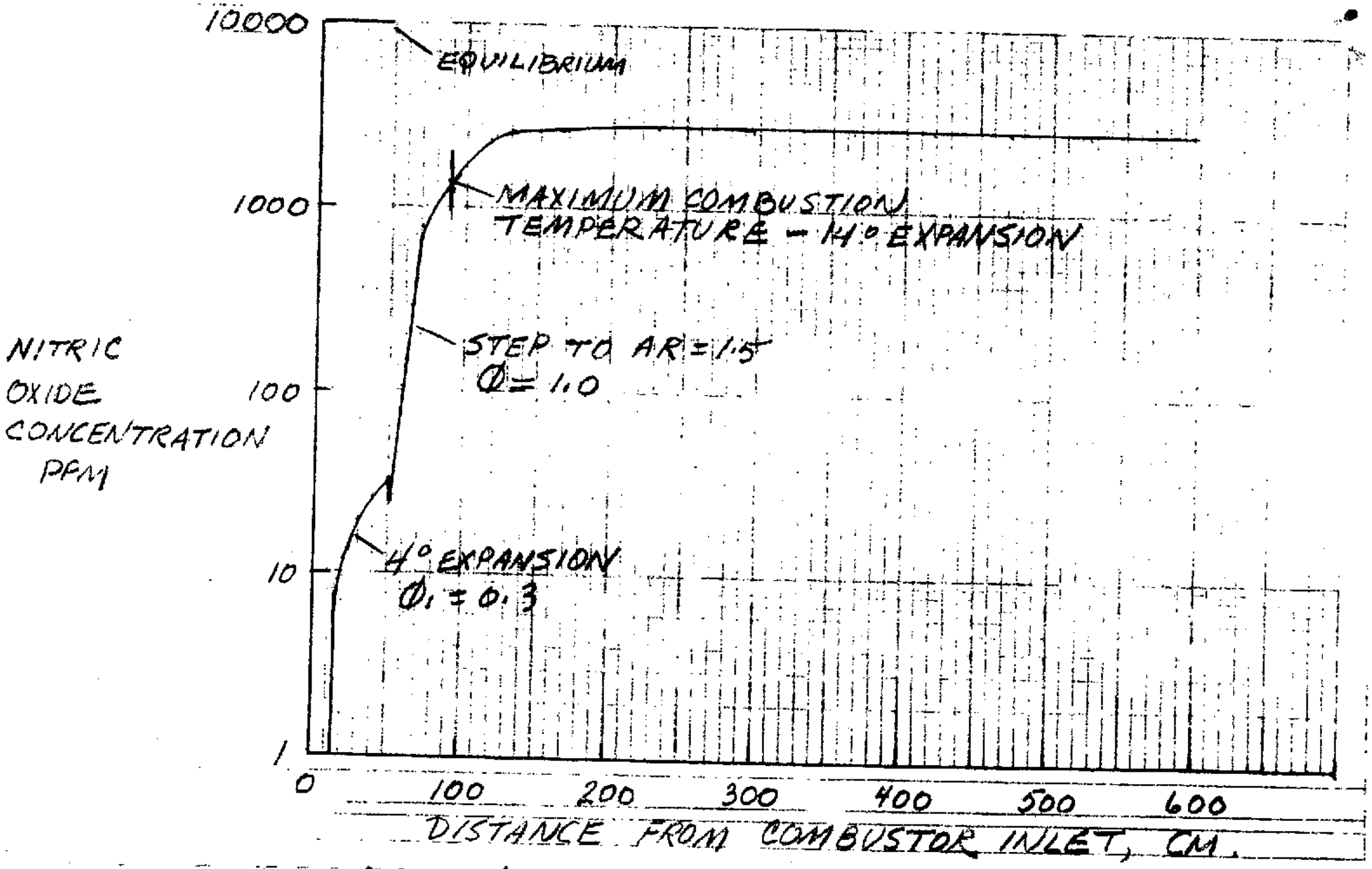


FIG. 2. CHEMICAL KINETIC CALCULATIONS OF NITRIC OXIDE FORMATION IN HYDROGEN FUELED SCRAMJET COMBUSTOR

(a) $M_\infty = 6$, $\emptyset = 0.65$

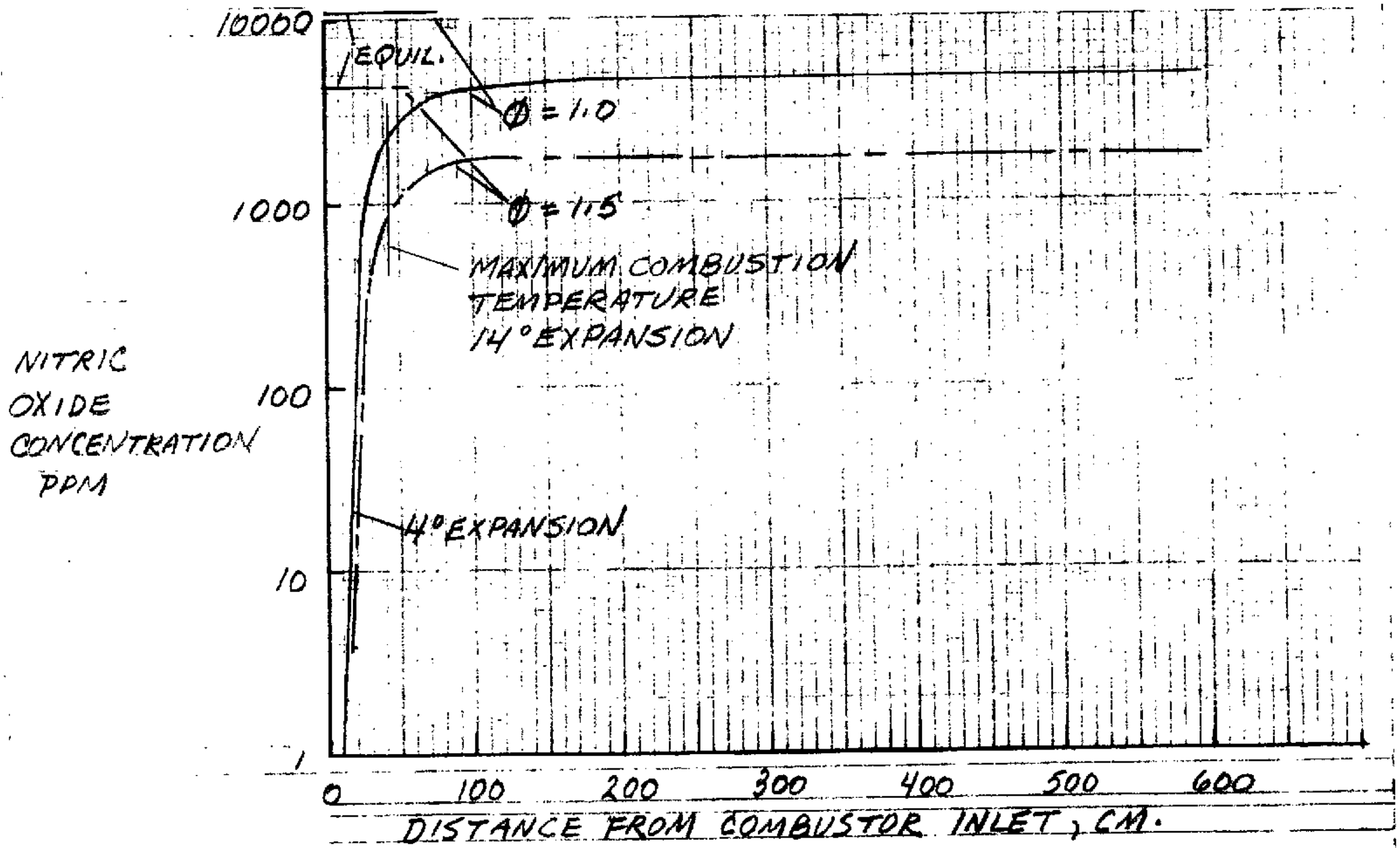


(b.) $M_\infty = 7$, $\Phi = 1.0$



(C) $M_\infty = 8$, $\phi = 1.0$

19



(d.) EFFECT OF EQUIVALENCE RATIO, $M_\infty = 10$

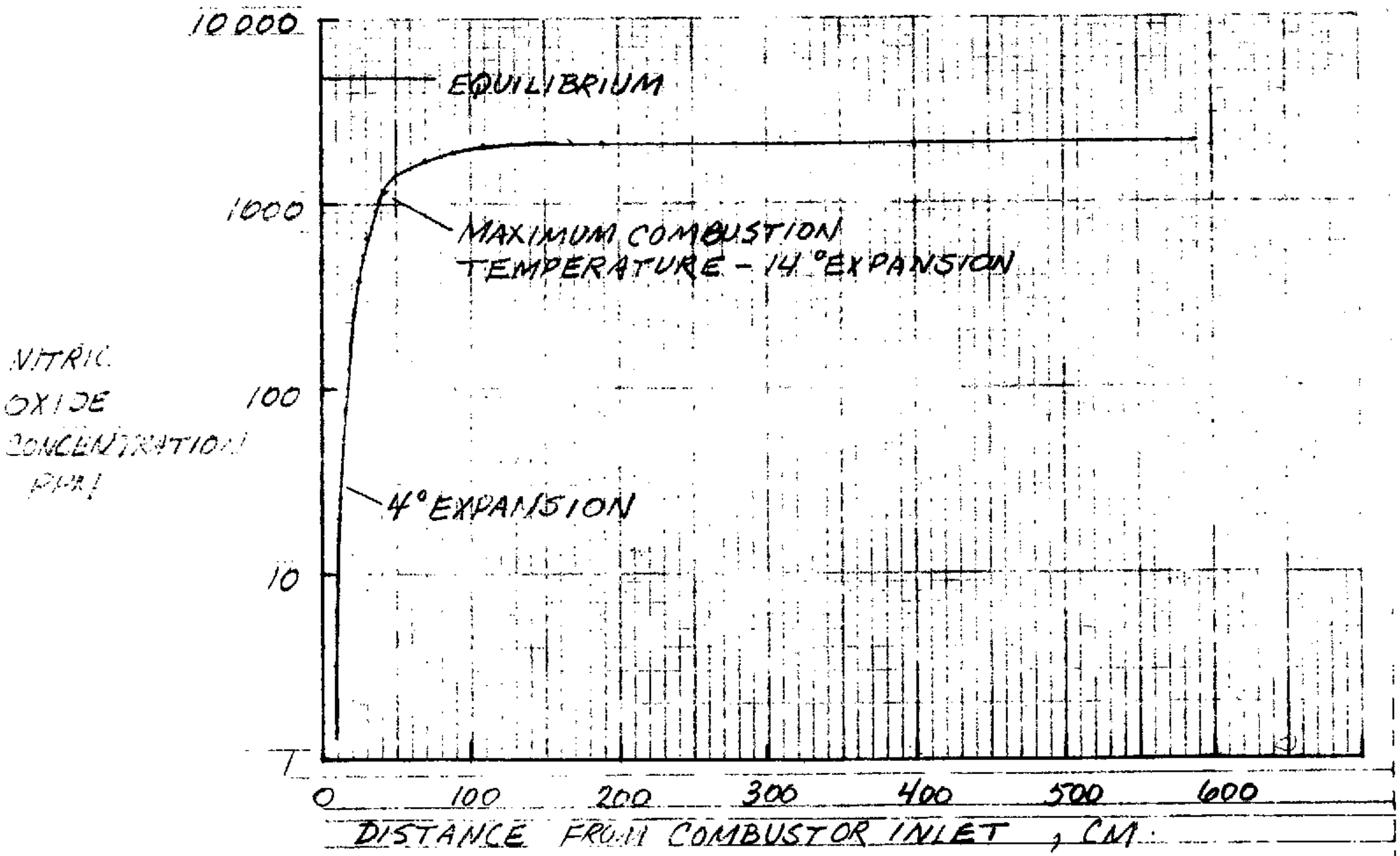
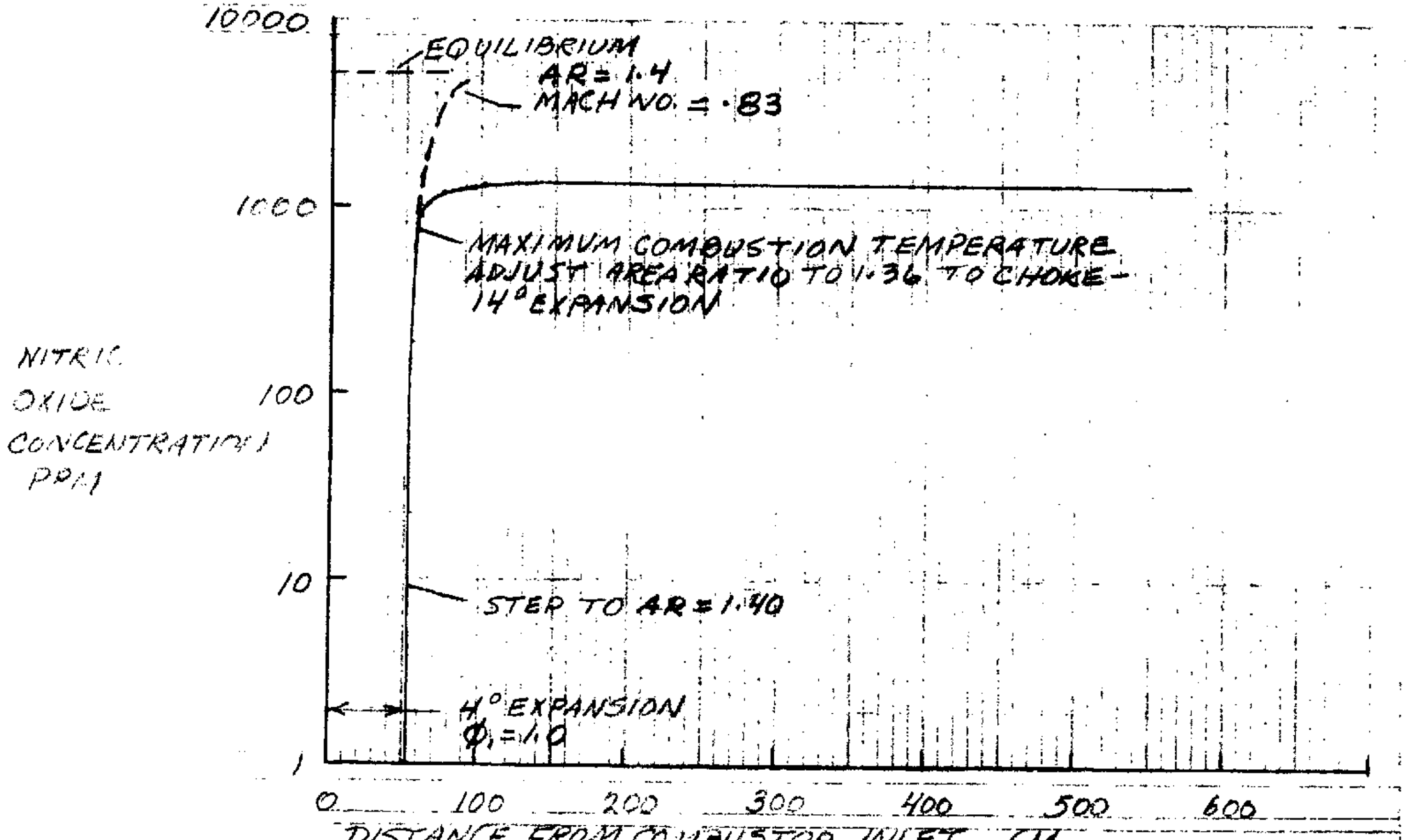


Fig. 2 (e.)

$M_\infty = 7.2$, $\Phi = 1.5$



(f.) SUBSONIC COMBUSTION, $M_\infty = 5$, $\Phi = 1.0$

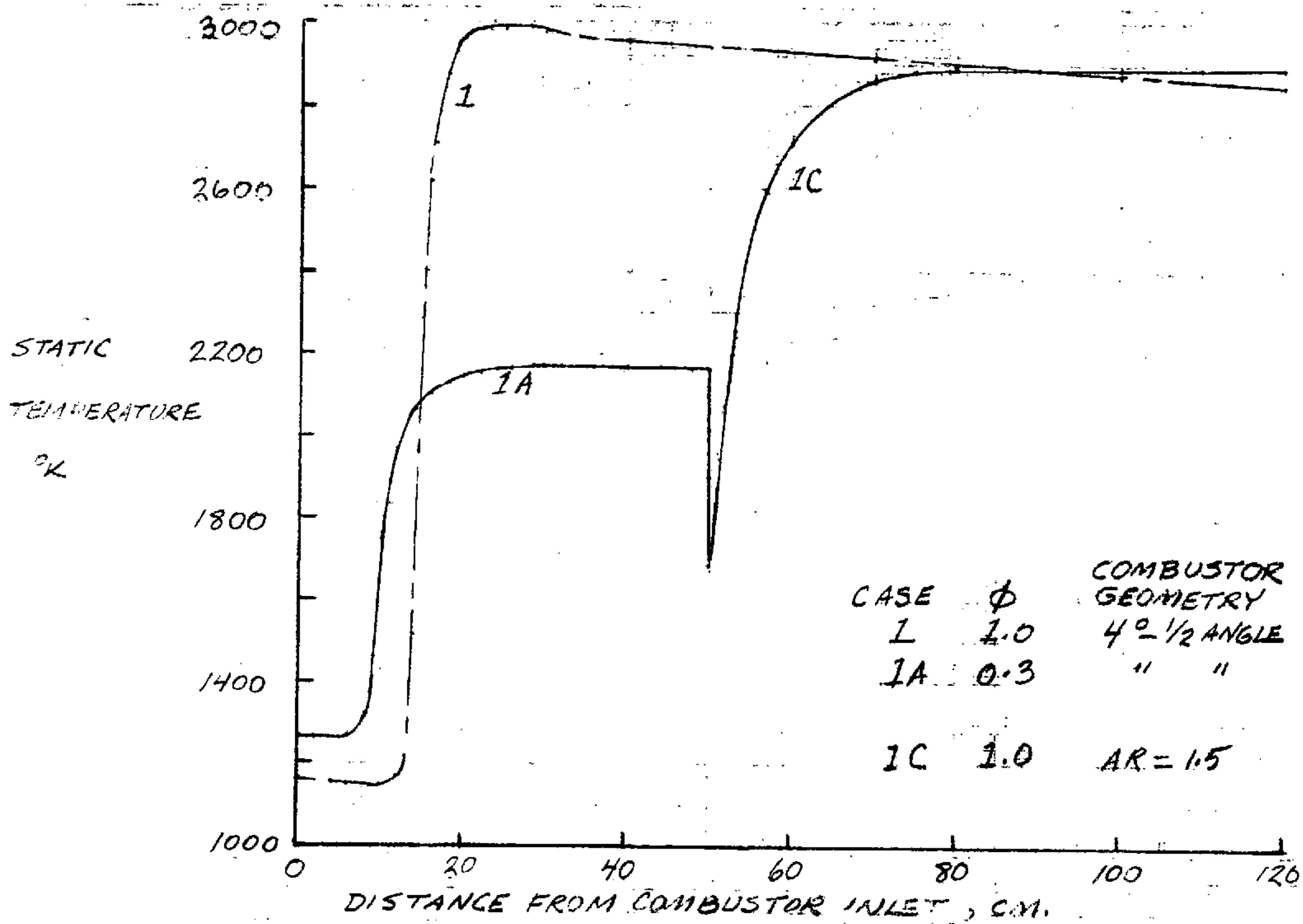


FIG. 3. EFFECT OF COMBUSTOR GEOMETRY AND FUEL STAGING ON REACTION TEMPERATURE - $M_\infty = 8$

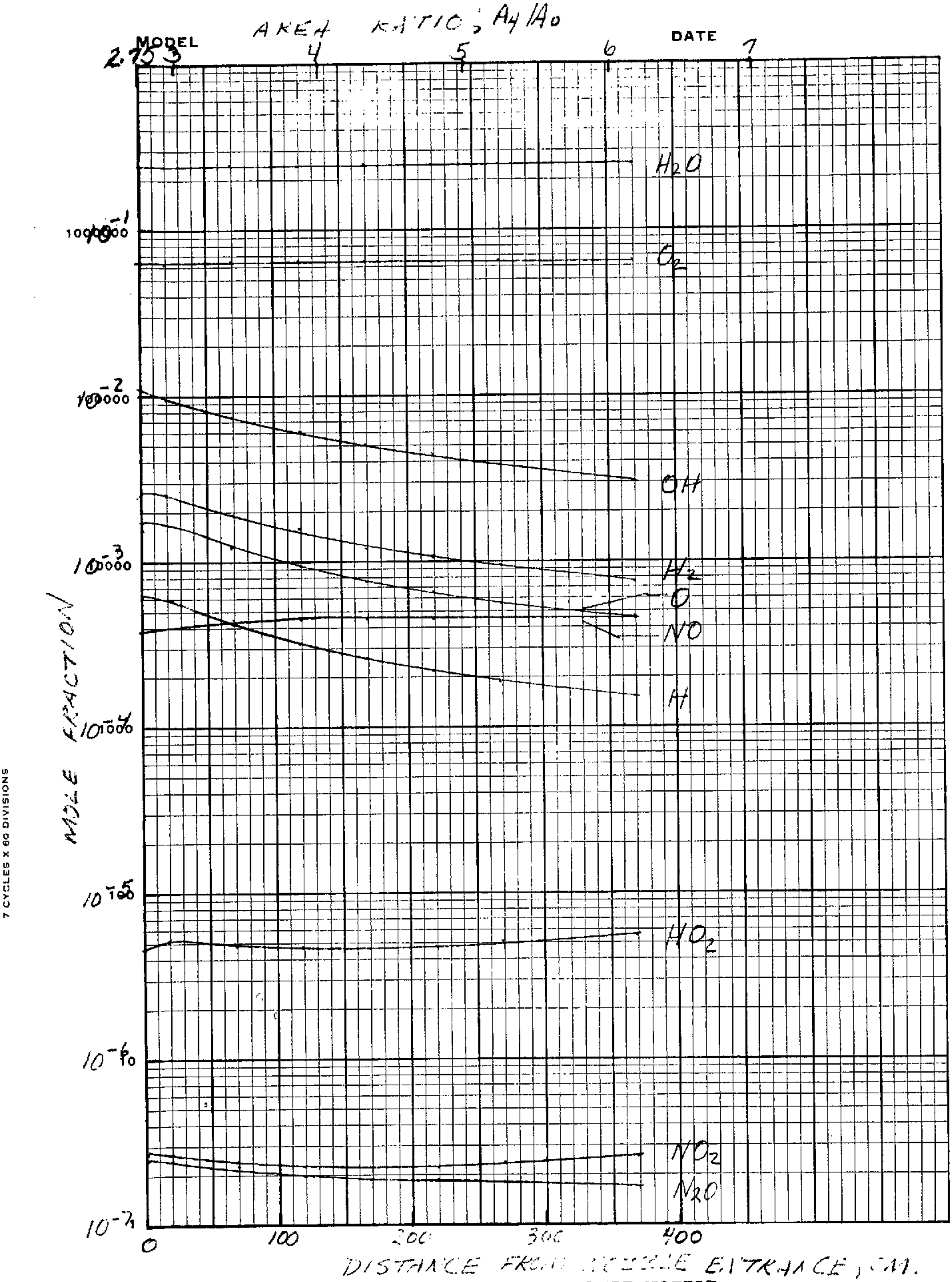
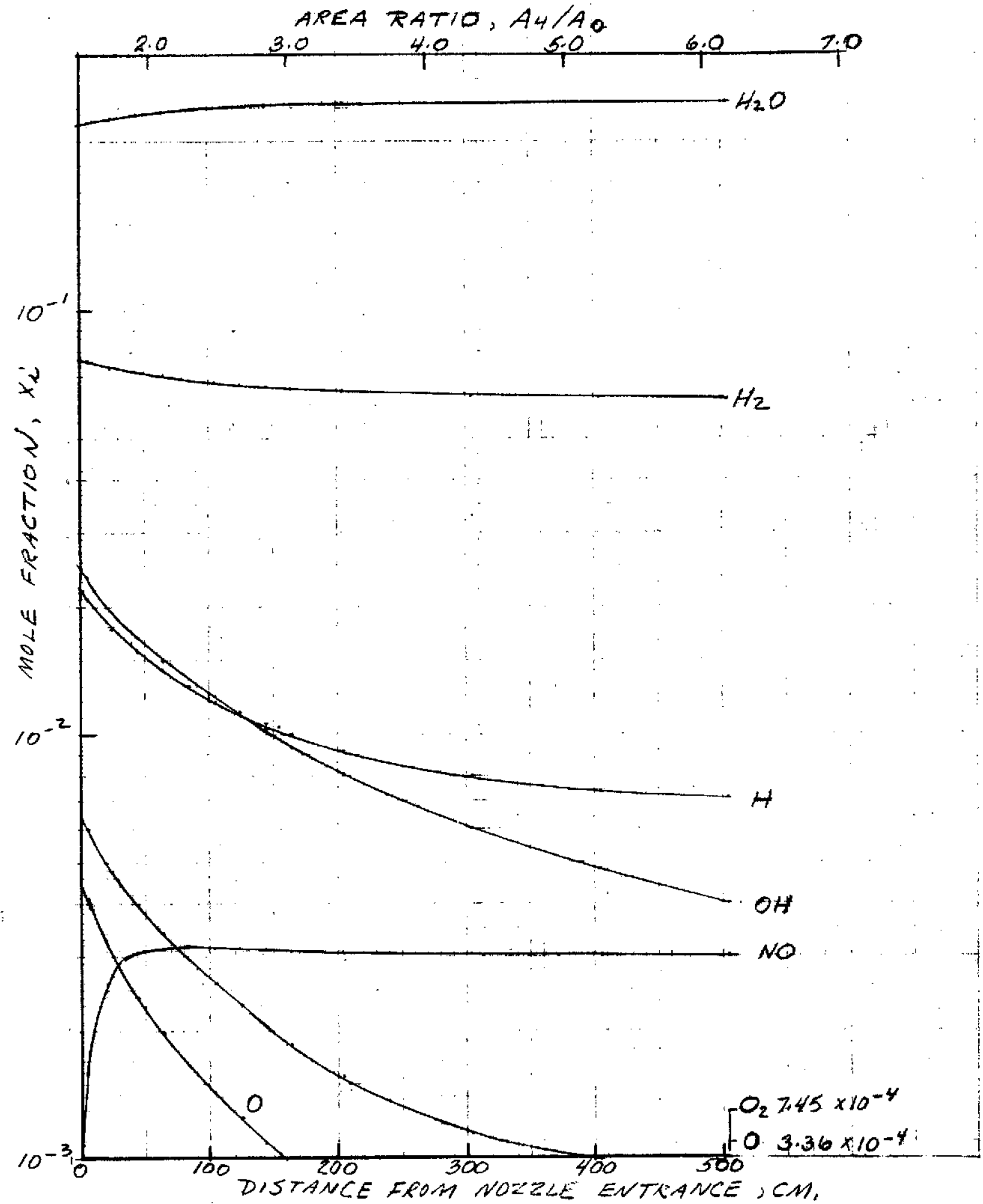
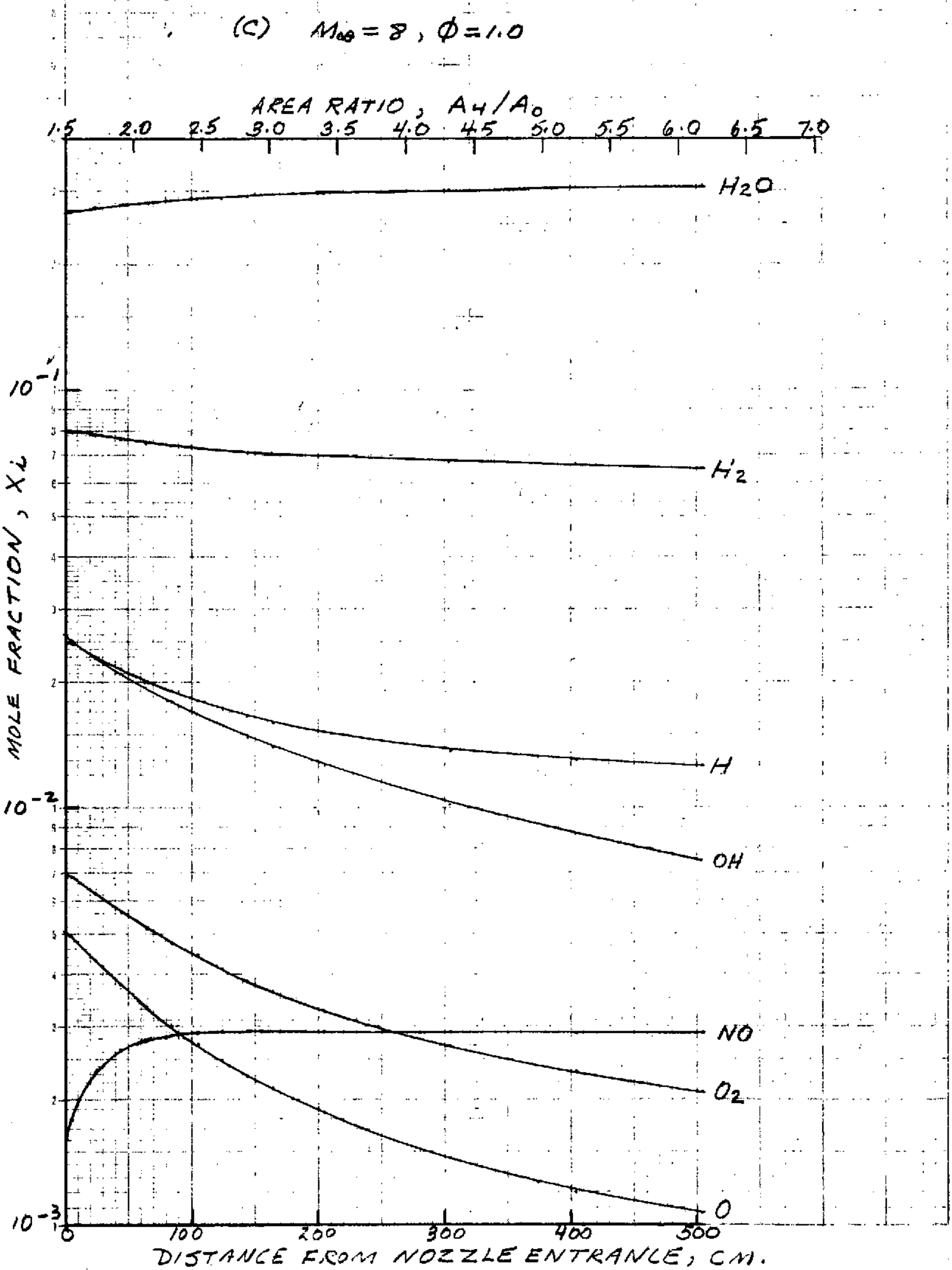


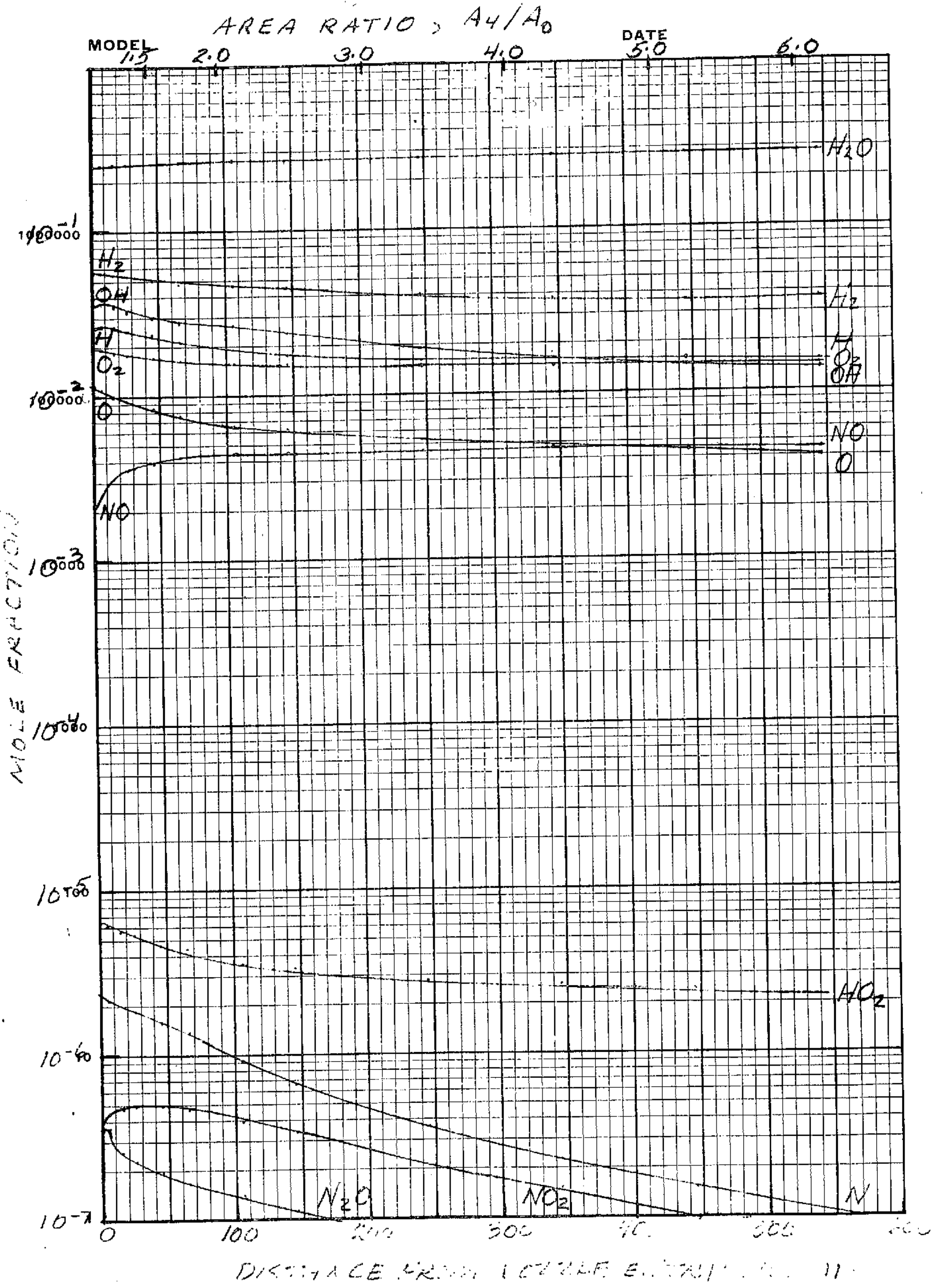
Fig. 4 KINETIC EXPANSION IN EXHAUST NOZZLE

(a) M = 6, Ø = 0.65

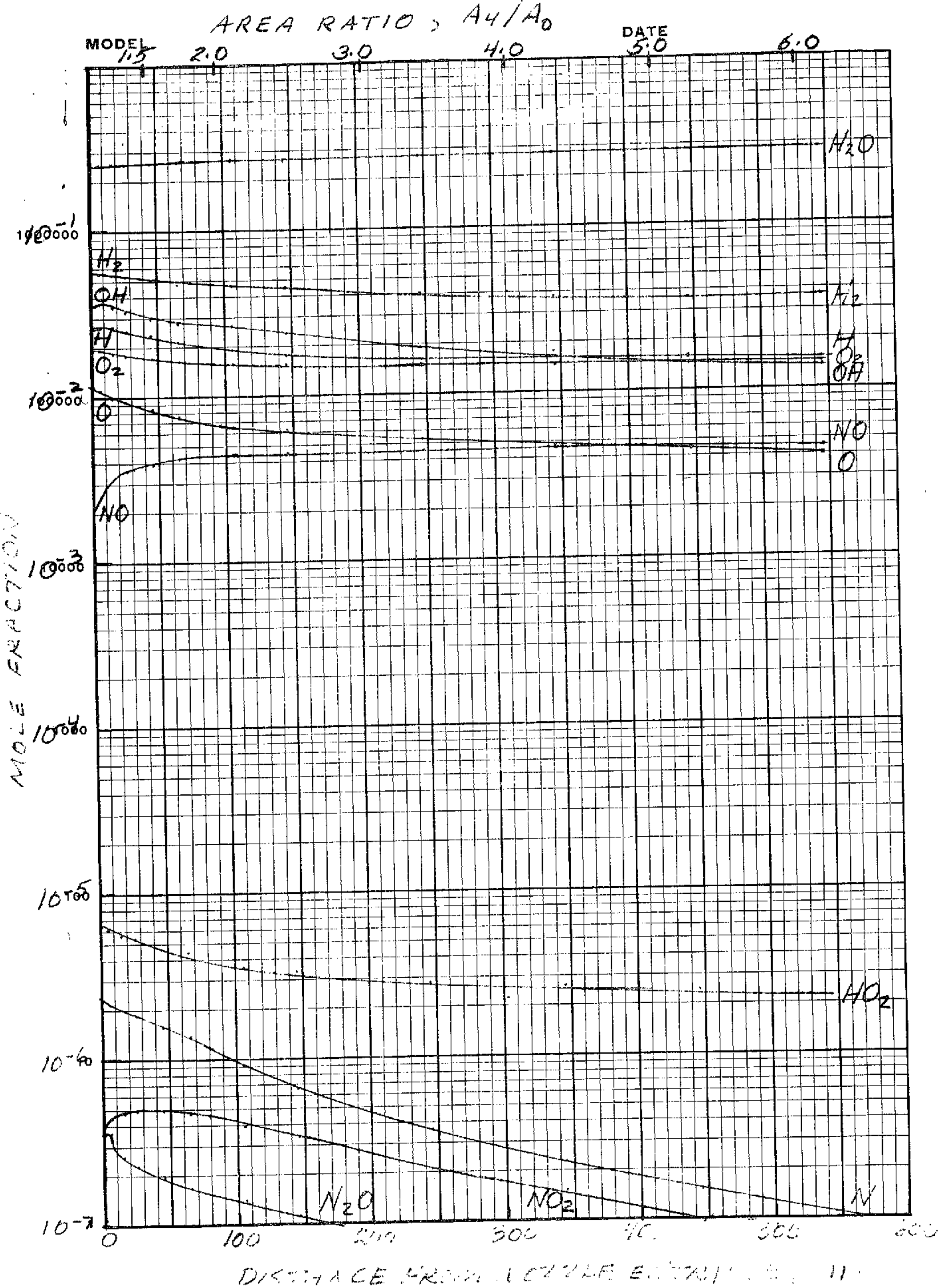
(b) $M_\infty = 7$, $\phi = 1.0$



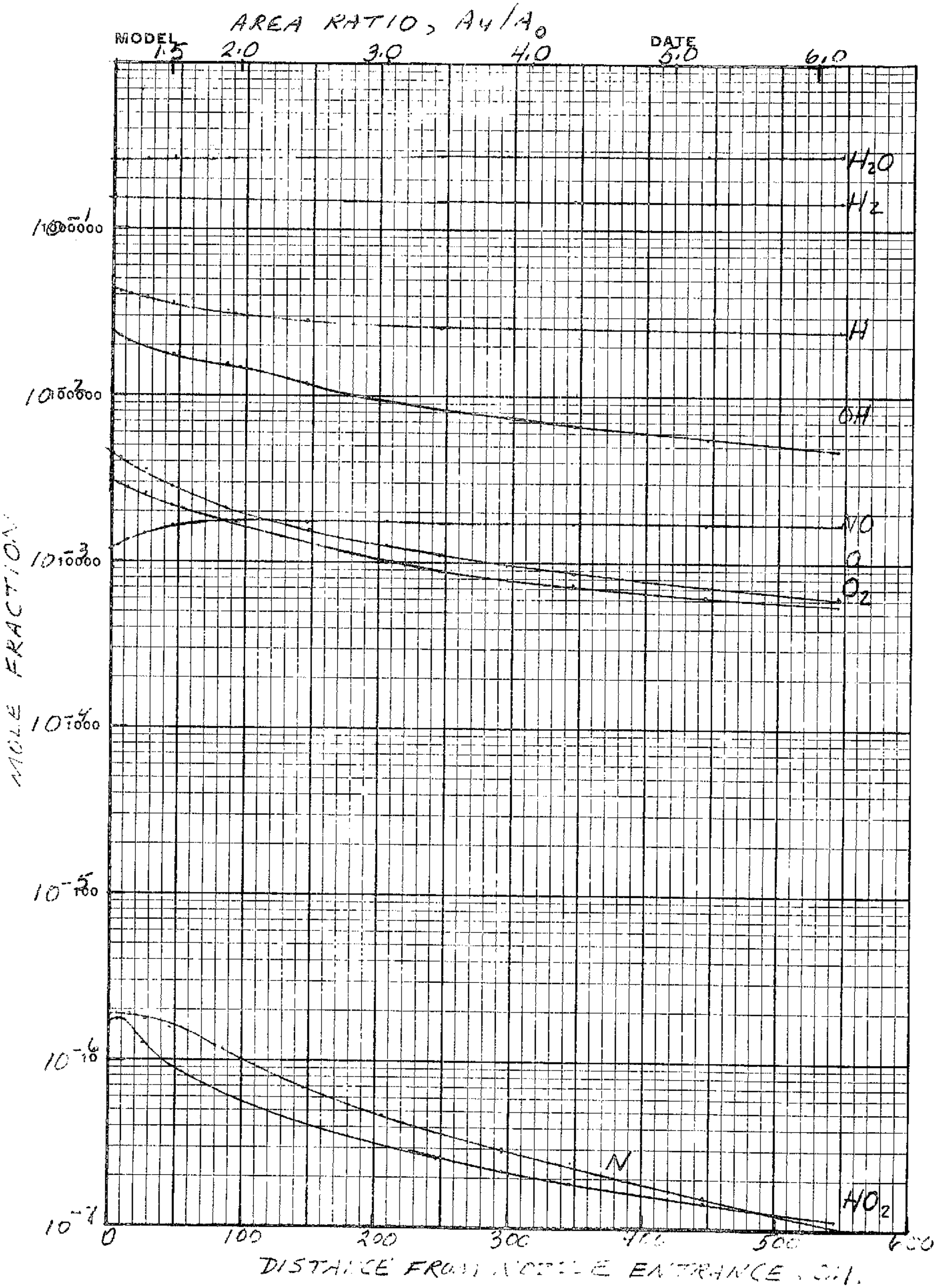

(C) $M_\infty = 8$, $\phi = 1.0$
AREA RATIO, A_4/A_0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
H_2O
10^{-1}
H_2
MOLE FRACTION, X_i
H
10^{-2}
OH
NO
O_2
O
10^{-3}
0
100
200
300
400
500
DISTANCE FROM NOZZLE ENTRANCE, CM.



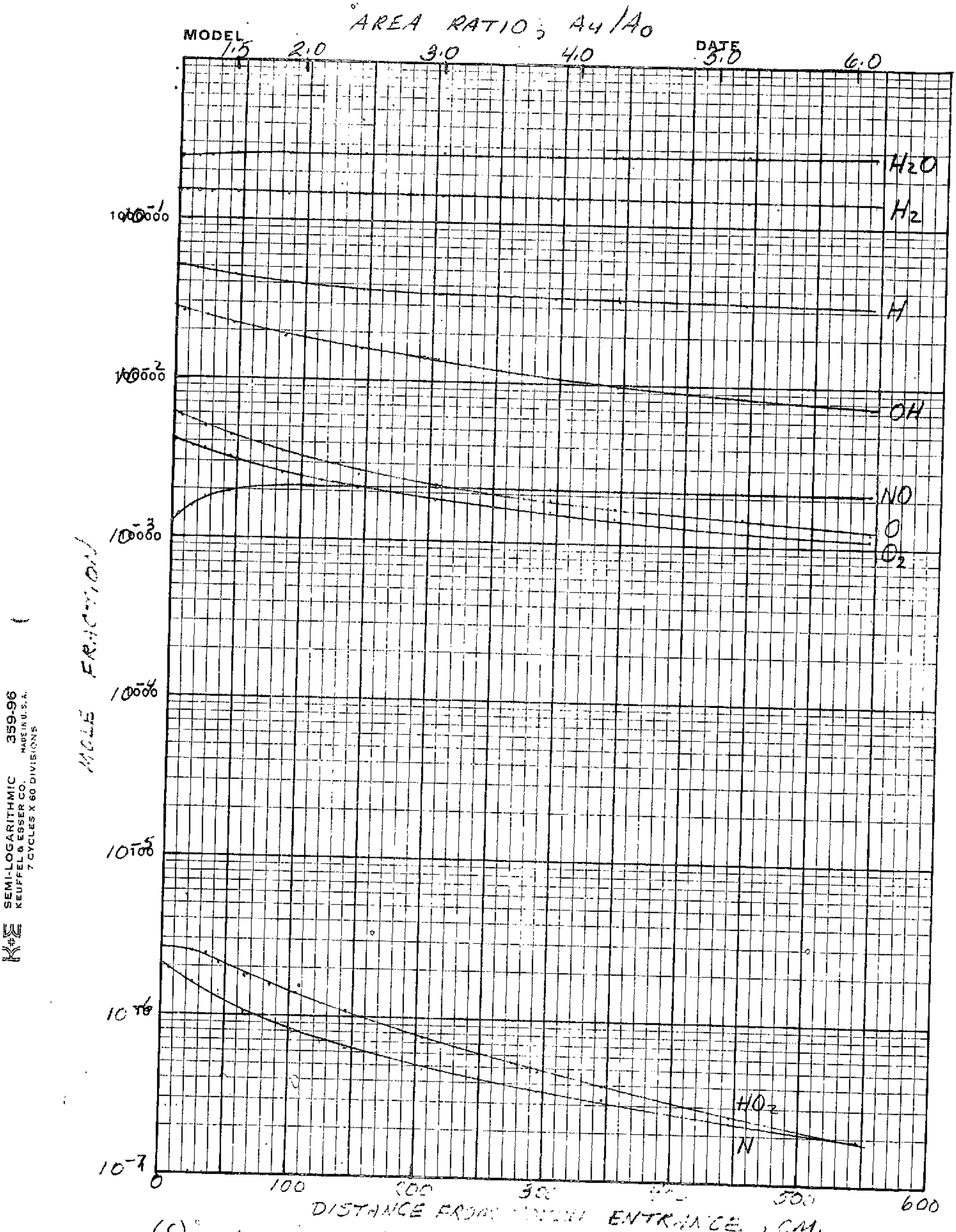
(d) $M_\infty = 10, \phi = 1.0$



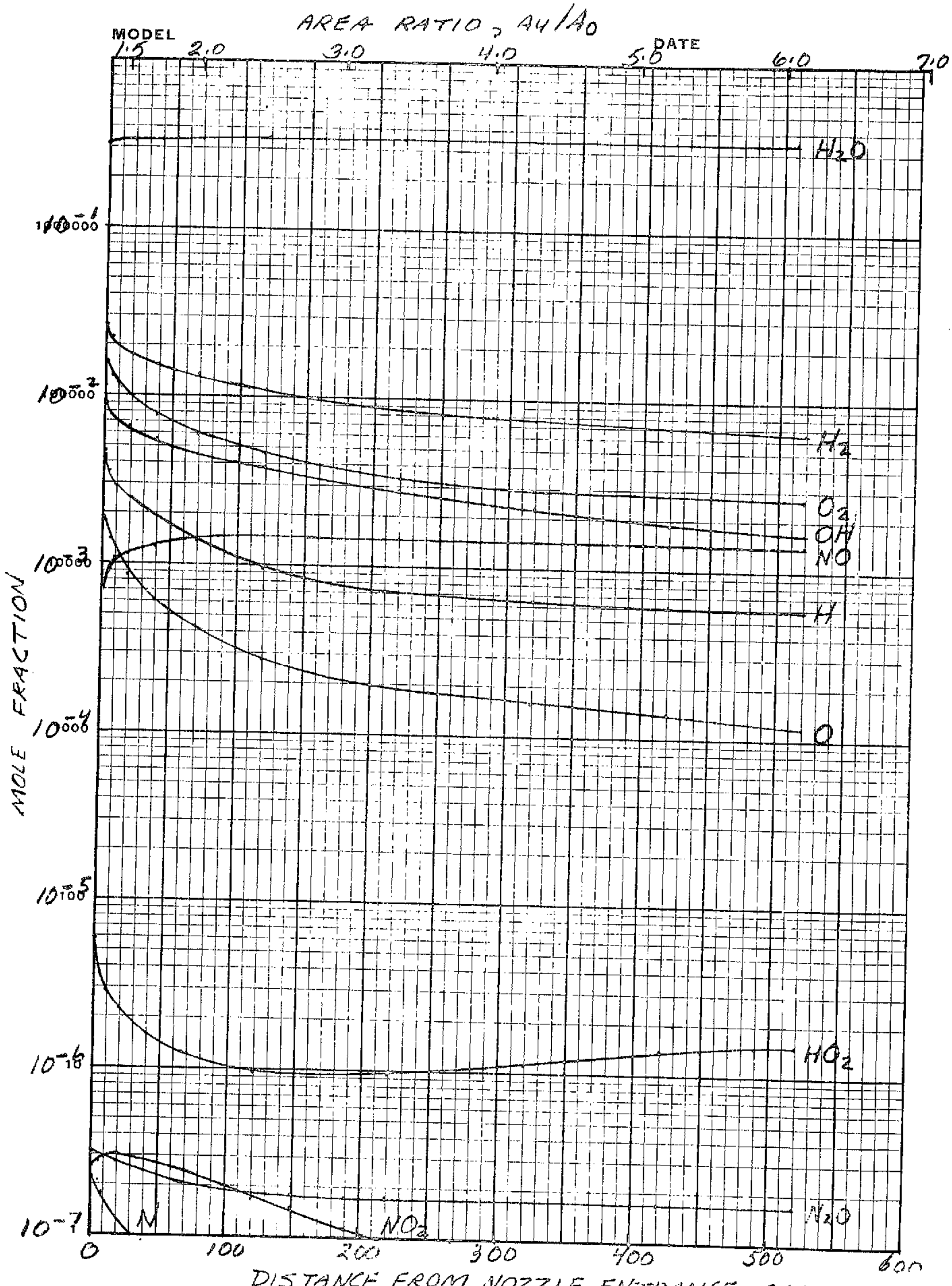
(d) $M_\infty = 10$, $\phi = 1.0$



(e) $M_\infty = 10$, $\phi = 1.5$



(f) $M_\infty = 12$, $\phi = 1.5$



(9) $M_\infty = 5$, $\Phi = 1.0$